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Predicting the Performance of Gaseous Air Cleaners: Measurements and Model Simulations from a Residential-Scale Pilot Study

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ABSTRACT

As part of an ongoing effort to evaluate the predictive capability of indoor air quality (IAQ) simulation tools, the National Institute of Standards and Technology (NIST) is evaluating the ability of the multi-zone IAQ model CONTAM to predict the effectiveness of different control strategies to reduce indoor concentrations of particle and gaseous contaminants. This report describes an evaluation of gaseous air cleaners and includes a literature review of gaseous air cleaning, development of an in situ air cleaner test method, determination of the performance of two gaseous air cleaners in a single room test house, and validation of CONTAM's ability to predict gaseous air cleaner performance. The literature review provides a summary of the available gaseous air cleaner technologies, including carbon adsorption, chemisorption, ozonation, and photocatalytic oxidation. Lack of gaseous air cleaner field testing protocols required the development of a test method using semi-real-time measurements and mass balance models. These test methods were used in a field study that involved a total of 23 experiments to evaluate the effectiveness of a portable carbon adsorption air cleaner and an in-duct chemisorption air cleaner to remove toluene from a single room test house for a range of environmental and operating conditions. Air cleaner removal efficiencies were similar for the two air cleaners and ranged from 26 % to 61 %. For the given conditions, these removal efficiencies were equivalent to air cleaner effectiveness rates of 69 % to 95 %, well above the effectiveness of infiltration and sorption to remove toluene from the test house. Of all of the operating conditions tested, only relative humidity appeared to have an impact on the in-duct air cleaner's performance. Five additional tests were completed to determine the ability of CONTAM to predict the performance of each air cleaner. Simulations were run with removal efficiencies determined experimentally, and the predicted concentrations were compared with concentrations measured in the five independent tests. Based on a statistical analysis, CONTAM proved to be an effective tool for predicting the impact of air cleaner performance in the well-mixed, single zone environment.

KEY WORDS: air cleaners, indoor air, VOC transport, field study, model validation.

INTRODUCTION

Residential and commercial gaseous air cleaning (GAC) technologies have not gained wide acceptance in the marketplace, in part due to the lack of rating methods, field performance data, and model simulation studies. Currently, there are no standard test methods available for gaseous air cleaners, and there is no system in place to rate the performance of these devices in the laboratory or field. For the most part, GAC performance data has been based on laboratory testing, which often involves high challenge concentrations, low airflow rates, single contaminant species, and controlled temperature and relative humidity (Silberstein, 1991; VanOsdell, 1994). Air cleaner removal efficiencies obtained under such conditions may not be representative of the air cleaner's performance in the field. Lack of field performance data has also hindered the ability to simulate GAC removal. Currently available air cleaner models use a first order removal rate that is based on a removal efficiency obtained in a laboratory test.

To obtain field data and predict the impact of air cleaner technologies on the indoor environment, NIST is conducting a study to 1) measure the impact of using air cleaners in single and multi-zone test houses, 2) determine important factors that affect air cleaner performance, and 3) determine the capability of the indoor air quality model CONTAM to predict the impact of different types of air cleaner technologies. To date, testing has been completed on the performance of particle filtration devices in a single zone (Emmerich and Nabinger, 2001) and a multi-zone building (Emmerich *et al.*, 2004). This report provides initial gaseous air cleaner testing and simulation data for a single zone test house. A field test protocol was developed to determine the toluene removal effectiveness of a portable room air cleaner with adsorption media and an in-duct air cleaner with chemisorption media. Environmental conditions, including building air change rates, were measured on a semi-real time basis to allow for calculation of all removal mechanisms including sorption on surfaces, exfiltration, and air cleaner removal. Air cleaner performance was determined two ways, including a direct upstream versus downstream concentration measurement and empirically with a single zone mass balance model. Results from these experiments were then used to evaluate the predictive capability of CONTAM.

LITERATURE REVIEW

Historically, gas-phase air cleaners have primarily been used in industrial applications with a limited number of contaminants at concentrations that are orders of magnitude greater than those found in non-industrial environments (ASHRAE, 2003). Similar technologies, however, are now being applied in commercial buildings, homes and other non-industrial environments. The following review provides background information regarding currently available gaseous air cleaner technologies for non-industrial environments with a focus on performance issues in the field. Although no standard test exists at this time for evaluating gaseous air cleaners, NIST has recommended that the following performance criteria be considered (Mahajan, 1987): 1) removal efficiency for specific contaminants; 2) lifetime of device and maintenance requirements; 3) sensitivity to relative humidity and temperature; and 4) the nature of any effluent products created by the device. These issues will serve as a guide in reviewing different air cleaner technologies.

Currently available non-industrial air cleaning devices use one or more of the following processes: adsorption, chemisorption, ozonation, and/or photocatalytic conversion. Of these removal mechanisms, adsorption has been the most widely used in non-industrial buildings (VanOsdell *et al.*, 1996). Adsorption is an exothermic process where organic vapor molecules are attracted to the surface of an adsorbent material and trapped in the material's pores ($< 2 \times 10^{-9}$ m diameter). A more effective adsorbent will have a large surface area per given mass, a higher volume of pores, and a similar polarity to the vapor being collected (Fisk *et al.*, 1987). The most frequently used adsorbent is activated carbon, however silica gels, activated alumina, zeolites, porous clay minerals, and molecular sieves are also used (Godish, 1989). Adsorbents are typically packed in a bed for VOC removal, but they may also be embedded in fabric filters or coated on surfaces of particulate filters. VOCs most likely to be removed by adsorption to activated carbon tend to be non-polar and have high boiling points, such as aldehydes, ketones, alcohols, alkylbenzenes, and halocarbons (Godish, 1989).

Removal efficiencies of gaseous air cleaners using adsorption technology have been reported to range from 0 % to > 90 % (Weschler *et al.*, 1994; Shaughnessy *et al.*, 1994; Daisey and Hodgson, 1989). Contaminant removal is largely a function of contaminant type and mass of adsorbent in the cleaner. For example, Shaughnessy *et al.* (1994) tested 9 different air cleaners with activated carbon for three contaminants. A few had limited success removing formaldehyde, and most were able to remove nitrogen dioxide to some extent. However, none removed carbon monoxide. Daisey and Hodgson (1989) confirmed that the removal rate of six VOCs (*n*-heptane, toluene, dichloromethane, tetrachloroethylene, hexanal, and 2-butanone) was higher when more mass of adsorbent was present.

An air cleaner using activated carbon or similar material is merely storing contaminants on the adsorbent material and thus requires maintenance to regenerate the adsorbent or replace the media. The lifetime of a particular adsorbent is often measured by its 10 % breakthrough time, *i.e.*, the time it takes the adsorbent's effluent concentration to reach 10 % of the influent concentration. VanOsdell (1996) reported 10 % breakthrough times ranging from 6.3 h to 38 h for VOC concentrations on the order of 40 mg/m^3 (10 ppm(v)). This range increased to 13.3 h to 344 h for VOC concentrations on the order of 4 mg/m^3 (ppm(v)). For toluene concentrations in the ppb range, Scahill et al. (2004) estimated 10 % breakthrough times to be 400 min/g to 500 min/g. In addition to challenge concentration, an adsorbent's capacity is also dependent on relative humidity, airflow velocity,

temperature, and presence of competing molecules (Fisk *et al.*, 1987). Several of these parameters are highly variable in the indoor environment, thereby making it difficult to predict when an adsorbent needs to be replaced or regenerated.

For physical adsorption, an increase of temperature will result in a decrease of adsorption capacity (Fisk *et al.*, 1987). For most residential applications, this effect is expected to be limited due to the relatively small variation in indoor temperature. It would be more of an issue for cleaning outdoor air, as is done for some commercial applications where the building mechanical ventilation would result in higher temperature variability of the filtered air stream. For both residential and commercial buildings, relative humidity can fluctuate considerably indoors and outdoors. This variation will have an impact on adsorption type air cleaners because water molecules can compete for adsorbent sites, even for non-polar adsorbents because the water condenses in pores. In the indoor environment, water is often at higher concentrations than other contaminants. Owen *et al.* (1995) looked at the effect of relative humidity on the performance of an adsorption air cleaner packed with activated granular coconut shell carbon. For relative humidities ranging from 0 % to 50 %, the 10 % breakthrough curves for a wide range of toluene challenge concentrations were not significantly affected. No significant reduction in 10 % breakthrough time was observed until the relative humidity was 75 %. At that point, 10 % breakthrough times tended to decrease with increasing relative humidity. For a toluene challenge concentration of 38 mg/m^3 (10.2 ppm(v)), the 10 % breakthrough time ranged from 61 h to 71 h for relative humidities less than or equal to 50 % and decreased to 16 h for a relative humidity of 82 %.

For simple adsorbent systems (no impregnated catalysts), there are no reactions with the sorbed contaminants creating harmful byproducts. However, there is the possibility of desorption of certain sorbed species when the air cleaner becomes saturated and/or the upstream concentration decreases or goes to zero. Since indoor environments are characterized by variable pollutant emissions due to intermittent sources (e.g., smoking, hobby activity, painting, etc.), the air cleaner may become a source of indoor air pollutants during low emission periods.

Chemisorption can extend the capabilities of adsorption through use of a reactive chemical coating on the sorbent surface. The resulting surface chemical reaction is effective at removing specific organic compounds. For example, formaldehyde is not removed well by activated carbon unless it is impregnated with a chemisorbent material (Godish, 1989). Types of chemisorption compounds include sodium sulfide, bromine, phosphoric acid, sodium carbonate, and metal oxides (Fisk *et al.*, 1987). Potassium permanganate is another chemisorbent that oxidizes contaminants primarily to carbon dioxide and water. Shaughnessy *et al.* (1994) tested the removal of formaldehyde using a four-stage filter with an adsorbent containing potassium permanganate. The filter was found to have a removal efficiency of 24 %. Air cleaners with carbon adsorbent systems were far less effective at removing formaldehyde in the study.

Increased temperature may enhance the removal capacity of contaminants when using an oxidative chemisorbent. The effect of relative humidity is less clear and depends on the chemistry between the chemisorbent and contaminant. Sometimes the interaction is positive, *e.g.*, the adsorbed water can enhance the oxidation reaction of potassium permanganate for hydrogen sulfide removal. For chemisorption of inorganic gases, the adsorption capacity of chemical sorbents also may vary with

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concentration, with the extent of the effect depending on the contaminant and on environmental conditions (temperature and relative humidity).

A drawback to oxidative chemisorption is the potential production of harmful byproducts resulting from chemical reactions. For example, hydrochloric acid may be produced when chlorinated hydrocarbons are oxidized (Godish, 1989).

Ozone generation is an air cleaning method that has generated significant controversy due to its preferential addition of ozone to the indoor environment and the potential byproducts of ozone reactions. Ozone is a very reactive compound that has been shown to reduce concentrations of certain VOCs, specifically aliphatic and aromatic alkenes (Boeniger, 1995). Weschler *et al.* (1992), found ozone to react with VOCs emitted by carpet including 4-phenylcyclohexene, styrene, and 4-vinylhexene. Concentrations of these compounds were reduced by as much as 90 % in the presence of ozone at concentrations of 0.055 mg/m^3 (28 ppb) to 0.086 mg/m^3 (44 ppb). Shaughnessey *et al.* (1994), however, tested two types of ozone generators and found them to have no measurable effect on removing formaldehyde and carbon monoxide at indoor air concentrations and only a small effect on removing nitrogen dioxide ($\approx$ 8 % removal efficiency).

As outlined in Boeniger's (1995) review of ozone generators, there are several issues associated with using this type of device. First, ozone reaction with many compounds often leads to the production of byproducts that are as or more harmful than the original pollutants. For example, Weschler and Shields (1997) have shown that ozone interactions with nitrogen dioxide and terpenes lead to increased levels of aldehydes, ketones, carboxylic acids, and organic nitrates. In addition, ozone is itself an indoor air irritant which can lead to upper respiratory distress for exposed occupants (Lippmann, 1989). Occupant exposure to ozone may be further increased due to the increased ozone generation rates at lower relative humidity levels, and the accumulation of ozone during periods of low contaminant concentrations (*i.e.*, periods of reduced ozone reactions) (Boeniger, 1995).

Finally, photocatalytic oxidation (PCO) is a more recently developed technology that has been shown to remove several classes of VOCs including: aromatics, nitrogen-containing ring compounds, aldehydes, ketones, alcohols, alkanes, chlorinated alkanes, terpenes, acetals, ethers, sulfur-containing organics, chlorinated ethylenes, and acetyl chlorides (Jacoby *et al.*, 1996; Alberici and Jardim, 1997; Blake, 1994). A PCO reactor uses a catalyst (typically TiO$_2$) activated by ultraviolet light (wavelength < 385 nm) to oxidize contaminants primarily to CO$_2$ and H$_2$O (Kagan,1993); however, intermediates sorbed to the catalyst and effluent byproducts have been reported (Jacoby *et al.*, 1996; Stevens *et al.,* 1998; Alberici and Jardim, 1997). Key steps in this process include transport of the contaminant to the catalyst, adsorption of the contaminant to the catalyst surface, and reaction of the contaminant with the activated catalyst (Jacoby *et al.*, 1996). Important factors affecting this process include challenge concentration, relative humidity, airflow velocity, temperature, and presence of competing molecules. In general, PCO air cleaners are characterized by low maintenance requirements and long service life due to the continuous regeneration of the catalyst during operation. There is the potential, however, for the catalyst to become poisoned during operation resulting in reduced contaminant removal.

Several studies have found relatively high removal rates for several types of VOCs at indoor air concentrations by PCO reactors (Alberici and Jardim, 1997; Stevens *et al.*, 1998; Lichtin and

Sadeghi, 1998; Jacoby *et al.*, 1996). For example, Alberici and Jardim (1997) used an annular, plug flow PCO reactor to determine the removal rates of 17 VOCs representing the following classes: ketones, alcohols, chlorinated alkenes, chlorinated alkanes, hydrocarbons, aromatics, ethers, acetals, and nitrogenated compounds. Eight of the 17 VOCs tested had destruction efficiencies greater than 90 %. In fact, all but four VOCs had destruction efficiencies greater than 65 %. Only isopropylbenzene, methyl chloroform, pyridine and carbon tetrachloride showed resistance to this removal technology. Stevens *et al.* (1998) showed nearly complete destruction of formaldehyde and acetone with four different types of PCO reactors. Similarly, Jacoby *et al.* (1996) used a PCO reactor that achieved 100 % destruction of benzene at steady-state indoor conditions.

Theoretically, a PCO reactor should completely convert contaminants to CO_2 and H_2O, however, intermediates sorbed to the catalyst and effluent byproducts have been reported. In general, the primary gas-phase byproduct in addition to CO_2 has been CO (Jacoby *et al.*, 1996). Intermediate products from the oxidation of organic compounds that sorb to the catalyst are likely to contain aldehydes, ketones, esters, and acids (Stevens *et al.*, 1998). For example, Jacoby *et al.* (1996) extracted malonic acid, phenol, benzoquinone, and hydroquinone from the catalyst following exposure to benzene. Alberici and Jardim (1997) observed conversion byproducts to be a function of contaminant residence time in the reactor. For most experimental flow rates, no byproducts were detected, however, at a higher flow rate of 0.06 m^3/h, byproducts were detected for t-butyl methyl ether, dimethoxymethane, and isoctane. Jacoby *et al.* (1994) completed several experiments at different operating conditions to identify the products formed by PCO reaction of trichloroethylene. The authors used an annular PCO reactor with TiO_2 catalyst and an 8 W fluorescent black light (spectral maximum at 356 nm). Reaction products included dichloroacetyl chloride, phosgene, CO_2, CO, and hydrogen chloride.

Intermediate products are typically sorbed to the catalyst and are generally not a health hazard to occupants. However, there have been reports of loss of catalyst reactivity due to the buildup of intermediate products. For example, Alberici and Jardim (1997) observed an initial (30 min) steady-state destruction efficiency of toluene at a concentration of about 2 x 10^6 μg/m^3 of 87 % to 92 %, followed by a later (150 min) steady-state destruction efficiency of only approximately 21 %. This loss in conversion was attributed to deactivation of the catalyst by adsorbed intermediates. For lower toluene challenge concentrations (about 6 x 10^4 μg/m^3), there was less catalyst deactivation.

For typical indoor air contaminant levels, a PCO air cleaner may be considered a "self-cleaning" device. Jacoby *et al.* (1996) observed the elution of carbon dioxide and carbon monoxide after turning off the challenge contaminant. This indicates the reactor is destroying residual sorbed contaminants including intermediates formed by reaction. Even in cases of severe catalyst poisoning, catalysts have been regenerated by washing the surface with hydrogen peroxide and exposure to a light source for one hour (Alberici and Jardim, 1997).

Several researchers have considered the impact of temperature and relative humidity on the performance of a PCO reactor. Lichtin and Sadeghi (1998) did not find the removal rate of benzene to vary significantly over a temperature range of 15 °C to 70 °C. According to the authors, the lack of impact of typical indoor temperatures on benzene's removal rate is consistent with photochemistry theory. PCO reactors must be operated in the presence of a certain amount of water vapor to maintain the performance of the catalyst. Alberici and Jardim (1997) found relative humidity in inlet air of

23 % to be adequate for maintaining the catalyst. However, too much water vapor can inhibit certain compounds' adsorption to the catalyst surface as noted by Jacoby *et al.* (1996). Obee and Brown (1995) used a monolith PCO reactor to investigate the impact of water vapor on the removal of formaldehyde, toluene, and 1,3-butadiene. For a given flow rate and UV intensity, the oxidation rates of all three test chemicals decreased with increasing relative humidity above 1000 ppm(v). The authors concluded that for relative humidity levels from about 15 % to 60 % and contaminant concentrations below 1 ppm(v), the PCO reactor removal rate would be first-order with respect to contaminant concentration.

Gaseous air cleaning is an emerging field, with several different types of air cleaners available. To date, however, performance data for these devices has only been collected in a laboratory setting. Thus, there is a need to understand GAC performance in the field under realistic conditions and relate this performance to laboratory results as well as predictive air cleaner models. To address some of these needs, NIST has developed a GAC field test method to study the performance of two different GAC devices. The initial tests were carried out in a single-zone test house with the following field performance factors being varied: indoor relative humidity, HAC operation, and room location for a portable type of air cleaner. Results from these tests were then used to evaluate the capability of the indoor air quality model CONTAM to predict the performance of these GAC devices and to determine the need for improved predictive air cleaner models.

EXPERIMENTAL METHODOLOGY

Test Facility and Instrumentation

The performance of the air cleaners was measured in a test house located in Gaithersburg, MD ($\approx$ 35 km NW of Washington, D.C.). A floor plan of the house with experimental equipment and sampling locations is shown in Figure 1. The test house was of typical residential, wood-frame construction and consisted of a single room with an attic. The conditioned space had a volume of 85 m^3 and a floor area of 37 m^2. A more detailed description of the test house and its heating and air conditioning (HAC) system is found in Emmerich and Nabinger (2001).

As shown in Figure 1, several variables were measured during a single experiment. Four sample locations were used including two inside the house (center of room and south wall), one in the attic (not shown), and one outdoors. At each sample location, relative humidity, temperature, and tracer gas concentration were measured on a semi-continuous basis. Toluene concentrations were measured at the room center and outdoor locations, as well as upstream and downstream of the air cleaner. Two types of air cleaners were tested including an in-duct model that was always installed in the HAC system, and a portable air cleaner that was located either in the center or corner of the room.
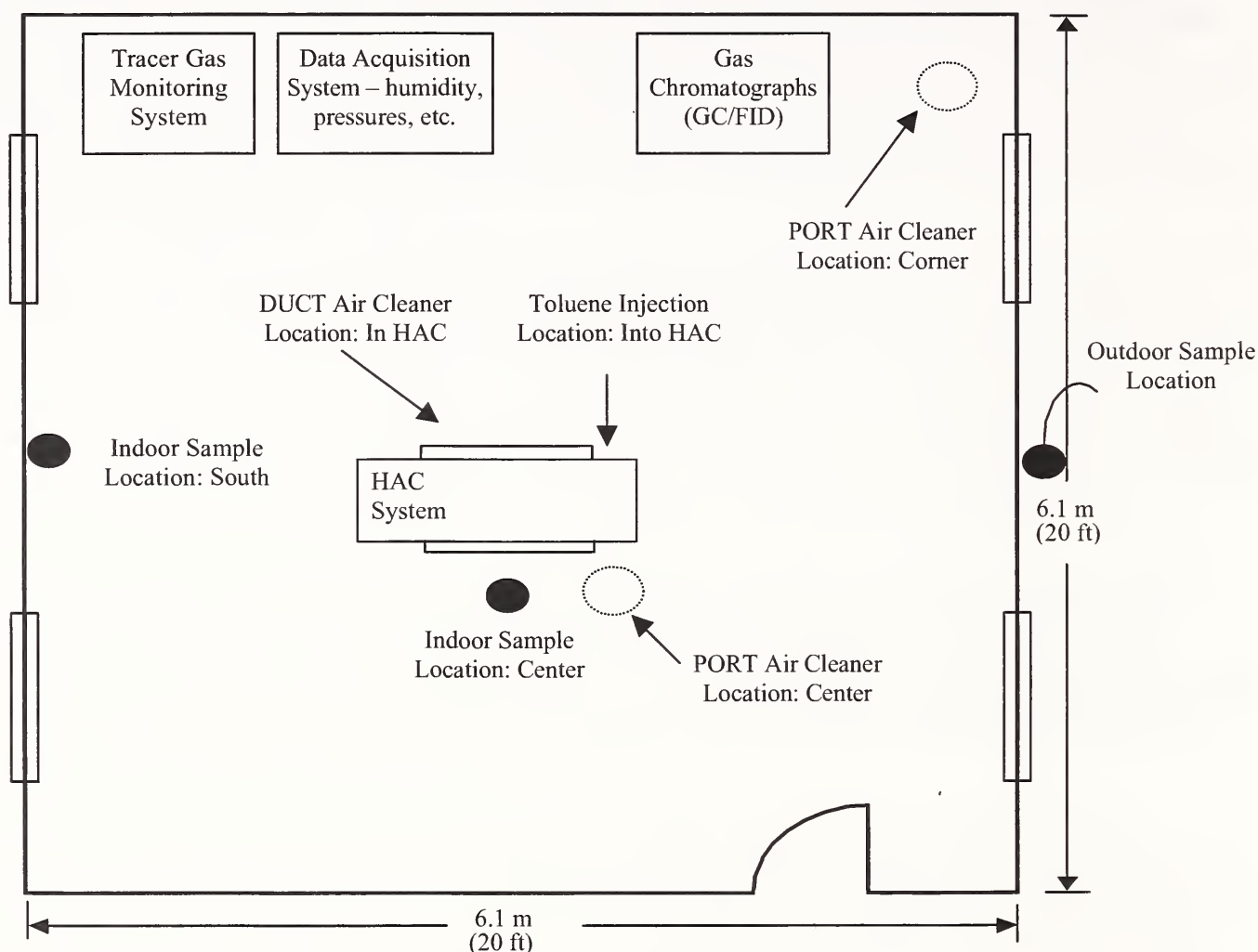

Figure 1. Test house floor plan with instruments and sample locations.

The house infiltration rate was determined by measuring the decay of sulfur hexafluoride (SF_6) as described in ASTM E 741 (ASTM, 2001). Every 6 h to 8 h, SF_6 was automatically injected into the house to an initial concentration of approximately 0.72 mg/m^3. Subsequent SF_6 concentrations were measured every 10 min at three indoor locations, the attic and outside with a gas chromatograph and electron capture detector (GC/ECD). Multiple indoor sample locations were used to ensure the variation in indoor SF_6 concentration among the indoor locations was within 10 %, thereby meeting the ASTM E 741 uniformity requirement. The measurement range of the GC/ECD was 0.03 mg/m^3 to 0.9 mg/m^3 with an accuracy of approximately $\pm$ 2 %. A linear regression of the natural logarithm of the SF_6 decay data was used to estimate the house air change rate every hour. The estimated uncertainty of the measured air change rates was approximately $\pm$ 10 %.

Indoor and outdoor environmental conditions were continuously monitored during the tests. Temperature was measured every minute in a central indoor location and outdoors with a thermistor (accuracy of approximately $\pm$ 0.4 °C). Relative humidity was also measured every minute in a central indoor location and outdoors using bulk polymer resistance sensors with an accuracy of $\pm$ 3 % RH. Wind speed and direction were measured with a sonic anemometer mounted 3.5 m above the test house roof. The anemometer was capable of measuring wind speeds from 0 m/s to 50 m/s ($\pm$ 5 %) with a resolution of 0.1 m/s. For wind speeds above 4.5 m/s, the wind direction had an accuracy of $\pm$ 5 %, but there was no specification of the accuracy for lower wind speeds.

Toluene was used as the challenge contaminant for testing the performance of the gaseous air cleaners. Toluene is a prevalent indoor air pollutant that is commonly studied in indoor air research. Toluene was injected into the house from a pressurized cylinder at a rate of 10 mg/h to 20 mg/h as regulated by a flow controller. For continuous injections, resulting steady-state concentrations in the house were 0.5 mg/m^3 to 2.0 mg/m^3. Toluene concentrations were automatically measured every 30 min using portable gas chromatographs equipped with flame ionization detectors (GC/FID). Samples were collected for 10 min at 0.006 m^3/h using an air sample pump and polytetrafluoroethlyene (PTFE) tubing. Measurement locations included at least one central indoor location, locations upstream and downstream of the air cleaner, and outside (see Figure 1). Samples were concentrated on the GC sorbent trap before injection into the GC column for separation and analysis. The GC/FIDs were calibrated to measure toluene concentrations ranging from 0.02 mg/m^3 to 2.0 mg/m^3 in the test house. Side-by-side tests were completed to detect any measurement bias between the instruments. The uncertainty associated with toluene concentration measurements was estimated to be approximately $\pm$ 5 %.

A photograph of each air cleaner is provided in Figure 2. The portable air cleaner (PORT) had a cylindrical design that consisted of a layer of zeolite sorbent, a high-efficiency particulate air (HEPA) filter, an activated carbon pre-filter, and an outer protective screen. The air cleaner's diameter was 40 cm, resulting in a 125 cm circumference through which air can be recirculated. The air cleaner airflow rate was measured using a shroud to enclose the air cleaner and then performing a traverse with a hot wire anemometer of a duct exiting the shroud. The maximum airflow setting corresponded to an average flow rate of 350 m^3/h ($\pm$ 12 m^3/h), which is considerably lower than the manufacturer reported airflow rate of 510 m^3/h. However, the configuration of the air cleaner used in these tests has changed since the manufacturer determined the higher airflow rate. In general, a lower measured flow rate than reported by the manufacturer is not uncommon, as similar discrepancies have been documented by other researchers (Shaughnessy *et al.*, 1994 and Daisey and Hodgson 1988).

The in-duct air cleaner (DUCT) consisted of a pleated fiber matrix impregnated with potassium permanganate in a 30 cm x 61 cm x 10 cm filter housing. The removal rate for this type of air cleaner is dependent on the duct airflow rate, which was continuously measured during tests with a hot wire anemometer with an accuracy of approximately ± 2 %. The average duct airflow rate was 378 m^3/h (± 17 m^3/h) with the air cleaner installed.
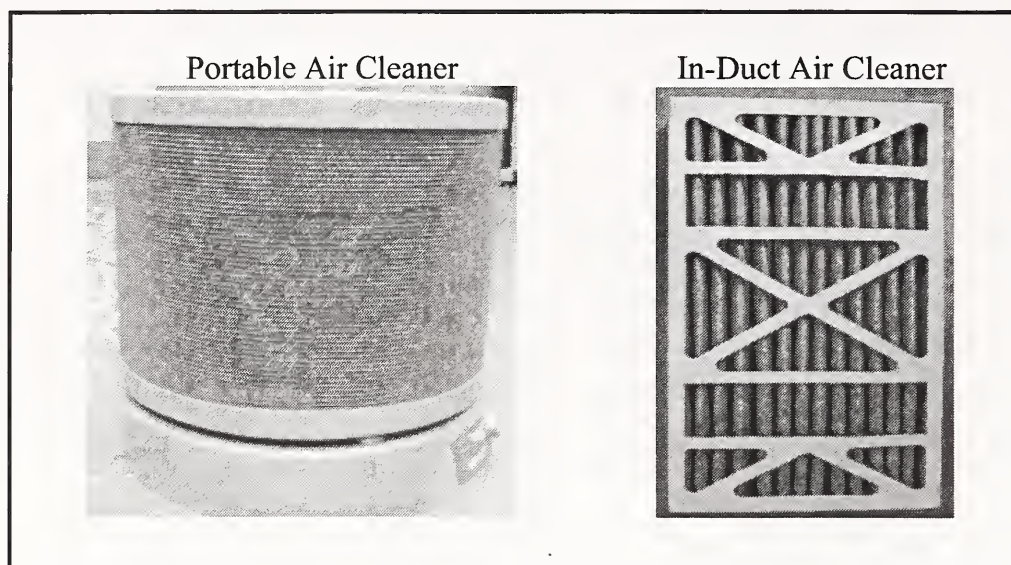

Figure 2. Photographs of air cleaners.

Experimental Design
Experiments were designed to identify important factors that affect air cleaner performance in the field. The scope of this work does not include air cleaner design parameters (*e.g.*, bed depth, packing density, type of adsorbent, residence time of air flow, *etc.*). The focus, rather, was on application parameters including relative humidity, HAC usage, and room location of the portable air cleaner. To vary the indoor relative humidity, a room humidifier was used to elevate the water vapor level for high humidity tests. This method increased the room relative humidity levels to a range between 41 % and 66 % for the different test conditions. To make this a discrete variable, a low humidity test included all experiments with relative humidity less than or equal to 40 % and a high humidity test included all experiments with relative humidity greater than 40 %. HAC usage was varied between on and off for the PORT air cleaner and heating and air conditioning for the DUCT air cleaner. Only the portable air cleaner location could be changed, and two positions were chosen including the center and corner of the room. To study these application factors, a 2^2 factorial design was used for the DUCT air cleaner and a 2^3 factorial design was used for the PORT air cleaner. The factorial designs are shown geometrically in Figure 3, where each corner represents an experiment with a unique combination of factors. The response variable for both designs was air cleaner removal rate of toluene, which was then converted to air cleaner performance.
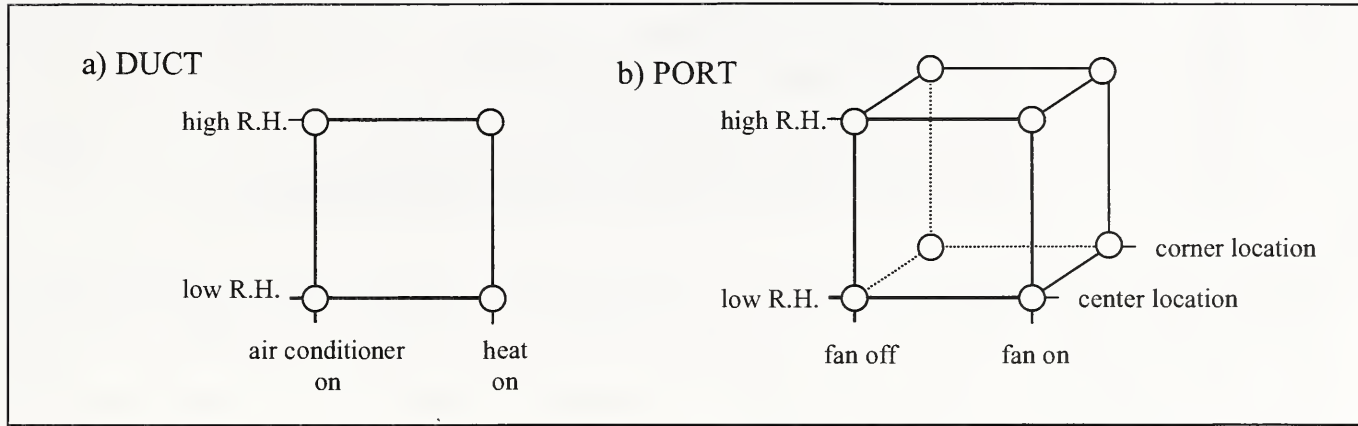
Figure 3. Factorial design for a) DUCT air cleaner and b) PORT air cleaner.

Data Analysis

Air cleaner performance was characterized by the effective cleaning rate (ECR) of each device, which is the product of the single pass removal efficiency and air cleaner airflow rate. Two methods were used to determine the air cleaners' single pass removal efficiency of toluene from the test house. For most tests, toluene concentrations were measured immediately upstream ($C_{upstream}$) and downstream ($C_{downstream}$) of the air cleaner. Using these measurements, the single pass removal efficiency (f_{dir}) of the cleaner may be directly calculated as:

$$f_{dir} = 1 - \frac{C_{downstream}}{C_{upstream}} \quad (1)$$

The second method used to calculate ECR was based on a two-phase single-zone mass balance model of the test house using a boundary layer diffusion controlled sink model to account for any adsorption/desorption to room surfaces (Axley, 1990):

$$M_z \frac{dC}{dt} = G + QC_{out} - QC + \frac{h\rho A}{K_p} C_m - h\rho AC - f_{mb} Q_{ac} C \quad (2)$$

$$M_s \frac{dC_m}{dt} = -\frac{h\rho A}{K_p} C_m + h\rho AC \quad (3)$$

where

M_Z	=	building mass of air (mg)
C	=	indoor VOC concentration (mg/mg)
t	=	time (s)
G	=	toluene emission rate (mg/s)
Q	=	outdoor air ventilation rate (mg/s)
C_{out}	=	outdoor toluene concentration (mg/mg)
h	=	film mass transfer coefficient acting over the sorbent surface (m/s)
ρ	=	air density (mg/m^3)

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A	=	sorbent surface area (m^2)
K_p	=	equilibrium partition coefficient (mg/mg)
M_s	=	mass of adsorbent material (mg)
C_m	=	toluene concentration in the sorbent (mg/mg).
f_{mb}	=	average single pass efficiency of the air cleaner (-)
Q_{ac}	=	airflow rate recirculated through the air cleaner (mg/s)

Experiments were completed in two phases. In the first phase, toluene was injected into the test house without the air cleaner operating until a quasi-steady-state concentration was reached (C_{ref}). In the second phase, the toluene injection continued but the air cleaner was turned on, and a new steady-state toluene concentration was achieved (C_{ctrl}). Assuming a constant Q, the associated steady-state solution of Equations 2 and 3 are as follows:

$$C_{ctrl} = \frac{G + QC_{out} + \dfrac{h\rho A}{K_p} C_{m,ctrl}}{Q + f_{mb}Q_{ac} + \dfrac{h\rho A}{K_p}} \tag{4}$$

$$C_{m,ctrl} = C_{ctrl} K_p \tag{5}$$

where:

C_{ctrl}	=	steady-state concentration of toluene with an air cleaner operating (mg/mg)
$C_{m,ctrl}$	=	steady-state toluene concentration in the sorbent (mg/mg), corresponding with time of C_{ctrl}.

Substituting Equation 5 into Equation 4 results in:

$$C_{ctrl} = \frac{G + QC_{out}}{Q + f_{mb}Q_{ac}} \tag{6}$$

For Phase I of the experiment when the air cleaner is off, Equation 6 may be simplified to:

$$C_{ref} = \frac{G}{Q} + C_{out} \tag{7}$$

where:

C_{ref}	=	steady-state concentration of toluene without an air cleaner operating (mg/mg).

To show the impact of using an air cleaner in this single zone environment, the air cleaner effectiveness was estimated. Nazaroff (2000) defined "effectiveness" as "the fractional reduction in pollutant concentration that results from application of a control device". At steady-state, air cleaner effectiveness may be directly determined as follows:

$$\varepsilon = 1 - \frac{C_{ctrl}}{C_{ref}} \tag{8}$$

where

ε =   air cleaner effectiveness (-).

EXPERIMENTAL RESULTS

A total of 23 experiments were completed with the portable (PORT) and in-duct (DUCT) air cleaners (see Table 1). Experiments were designed to evaluate the effects of HAC status, air cleaner location (PORT experiments), and room relative humidity. Due to some mechanical problems with the portable air cleaner, not all experiments of the factorial were completed. However, as discussed in a later section, none of the tested factors appeared to have a significant effect on the portable air cleaner performance in the test house. For each experiment, toluene removal rates due to infiltration, sorption, and air cleaning were determined. Of all the removal mechanisms, air cleaning was by far the most significant.

Table 1. Air cleaner experimental design.

	FACTORS			
PORTABLE	**R.H.**	**HAC**	**Location**	**# Expts.**
1	low	on	center	4
2	high	on	center	1
3	low	off	center	0
4	high	off	center	1
5	low	on	corner	2
6	high	on	corner	1
7	low	off	corner	1
8	high	off	corner	2
			TOTAL:	12
DUCT	**R.H.**	**HAC**	**Location**	**# Expts.**
1	low	on/ac	duct	3
2	high	on/ac	duct	2
3	low	on/heat	duct	4
4	high	on/heat	duct	2
			TOTAL:	11

Infiltration
The ventilation characteristics of the test house have been studied extensively and are reported elsewhere (Emmerich and Nabinger, 2000). Since that study, there have only been minimal changes to the building envelope such that much of the previous characterization work was not repeated for this study. Emmerich and Nabinger's (2000) work included fan pressurization tests, yielding an air change rate of 7.3 h^{-1} at 50 Pa and an effective leakage area of 140 cm^2 at 4 Pa. Figure 4 shows infiltration rates from Emmerich and Nabinger (2000) as a function of indoor outdoor temperature difference for wind speeds less than 0.5 m/s. A sample of infiltration rates for similar weather conditions from this study were added to Figure 4. As expected, the more recent infiltration rates follow the previous trends reasonably well.

The average infiltration rates measured during each air cleaner test are summarized in Tables 2 and 3 and ranged from about (0.1 ± 0.02) h^{-1} to (0.5 ± 0.05) h^{-1}. Without considering adsorption losses, these air change rates correspond to system time constants (τ) of 9 h to 2 h, respectively. Assuming

constant conditions, a reasonable estimate of C_{ref} (in Equation 7) would occur at $t > 3\tau$, about 6 h to 27 h.
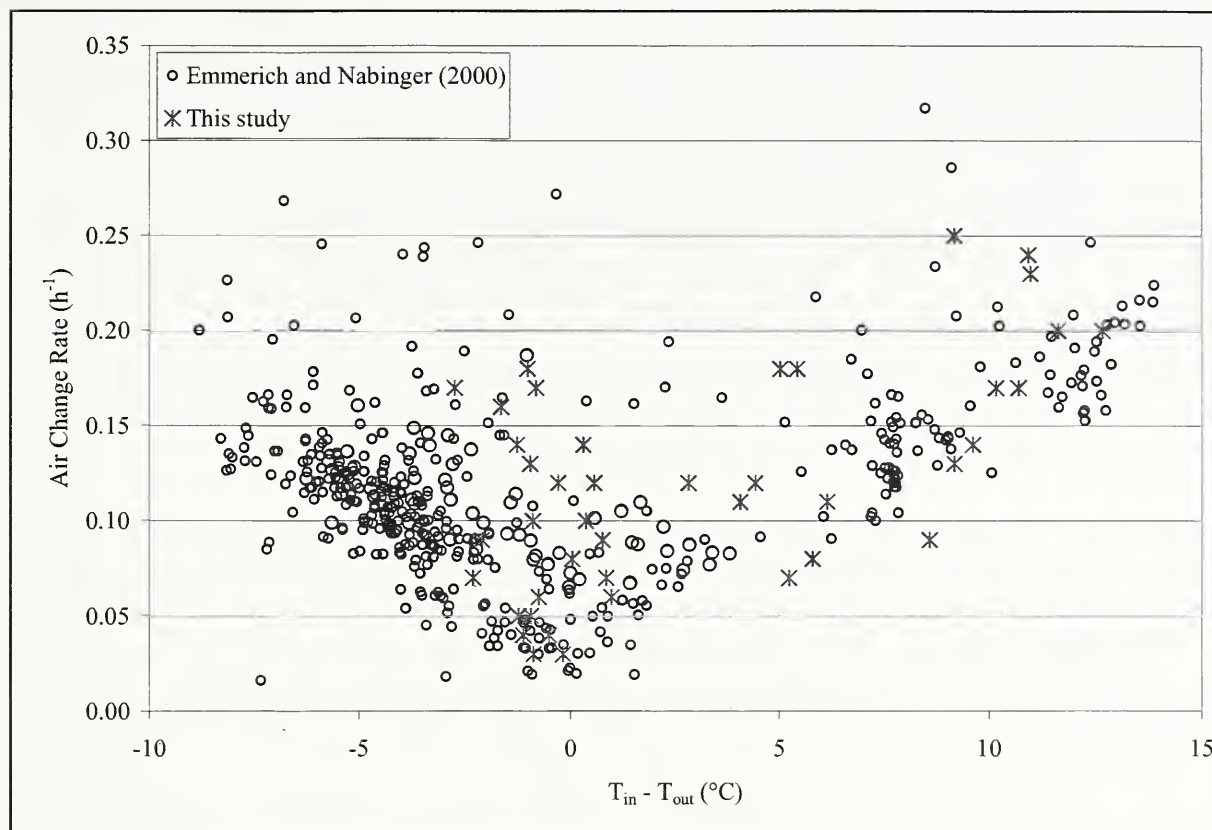

Figure 4. Infiltration rates measured at the test house as a function of indoor/outdoor temperature difference for wind speeds < 0.5 m/s.

Sorption
As shown in Equations 2 and 3, the mass balance of the single zone test house included terms to account for contaminant losses to surfaces as well as contaminant desorption from surfaces. As shown in Equations 6 - 8, it was possible to estimate air cleaner removal rates without knowledge of sink parameter values by using measured steady-state concentration values (C_{ctrl} and C_{ref}). As a result, sink values were not critical to the experimental determination of air cleaner performance. However, sink parameters were needed for the simulation phase of this work when steady-state conditions did not exist.

The first phase of each air cleaner experiment was used to predict the impact of sinks on toluene removal within the house. The variables specific to sink removal include the mass transfer coefficient (h), the chemical/material partition coefficient (K_p), area of the sink (A), and the mass of the sink (M_s). Since the sink model in Equations 2 and 3 is based on first principles, it is possible to estimate values of h, A and M_s using physical parameters. For example, the mass transfer coefficient may be estimated using equation 3.17a of Axley (1990):

$$h = Sh\left(\frac{D_{tol-air}}{L}\right) \quad \text{for Re} < 500\ 000 \tag{9}$$

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where:

Sh	=	average Sherwood number
		$Sh = 0.664\,Re^{\frac{1}{2}}\,Sc^{\frac{1}{3}}$ (10)
Re	=	effective Reynolds number
Sc	=	Schmidt number (≈ 1.0)
$D_{tol\text{-}air}$	=	gas diffusivity (m^2/s)
L	=	effective length of adsorbent surface (m)

Using Equation 9, the calculated mass transfer coefficient (h) for toluene in the test house was estimated to be 0.068 m/h. While this value of h is similar in magnitude to those reported by Axley (1990), it is at least two orders of magnitude smaller than deposition velocities seen in other studies (Nazaroff and Cass, 1986; Morrison and Nazaroff, 2002). Values of A and M_s may be estimated based on the surface area of primary adsorbent surfaces (painted gypsum board walls and ceiling) in the test house. Based on a wall and ceiling area of approximately 100 m^2 and a gypsum board density of 10 kg/m^2 (Axley, 1990), the mass of sorbent material was 1000 kg.

The remaining sink parameter (K_p) was estimated empirically using the mass balance equations for the first phase of each air cleaner experiment (*i.e.*, during toluene build-up with no air cleaner operating). Due to the dynamic nature of the test house conditions (*e.g.*, changing air change rate, *etc.*), the mass balance solutions were solved numerically. The partition coefficient was estimated using a best-fit solver routine in Microsoft Excel™. The curve fitting routines were based on the Generalized Reduced Gradient (GRG2) nonlinear optimization code (Lasdon *et al.*, 1978). It is also possible to find partition coefficients (K_p) for given contaminants and adsorbents in the literature (Zhang *et al.*, 2001). However, these values are for specific materials and may not completely reflect the materials present in a given building. Zhang *et al.* (2001) reported a partition coefficient of 941 m^3-air/m^3-gyp (1.5 mg/mg) for toluene and unpainted gypsum board.

Due to the relatively small surface area to volume ratio (1.5 m^{-1}) for the test house, the impact of sinks was expected to be relatively small compared to the impact of ventilation and air cleaning. Based on 22 of the 23 air cleaner tests, the best estimate of K_p was on the order of 1 x 10^{-5} mg/mg. As shown in Equation 3, K_p is coupled with M_s, so a more meaningful number to report is their product of 0.01 kg. Comparing this value with the total mass of air in the house (100 kg), results in an impact of 0.01 %.

Although the predicted value of K_p was several orders of magnitude lower than the literature value of 1.5 mg/mg, it is not that surprising. First, the literature value is for unpainted gypsum board, which would likely have a higher sink potential than gypsum board that is painted. Also, the estimated mass of the sorbent may be too high, resulting in a lower estimate of K_p due to their coupling in the mass balance equation. Finally, estimating sink parameters during loading conditions (i.e., toluene source on) is difficult. Any uncertainty in the source emission rate will have a significant impact on the sink parameters. In any case, the relative impact of sorption on the toluene concentration in the test house was quite small compared to the removal by ventilation and air cleaning.

Air Cleaner Results

Portable Air Cleaner

The single pass removal efficiency for the portable air cleaner was measured directly using upstream and downstream measurements and using the mass balance approach (see Table 2). For direct measurements, the average removal efficiency (f_{dir}) was 70 % (SD: 6.6 %) and ranged from 59 % to 77 %. The mass balance approach resulted in an average removal efficiency of 55 % (SD: 9.0 %) and had a range of 43 % to 61 %. Ideally, these approaches should yield the same result, however, the removal efficiencies determined with the mass balance were always lower than those measured directly, with the difference often greater than the associated uncertainties. One would expect the mass balance method to be more representative of the impact of the air cleaner in the room and the direct measurement to be more similar to the laboratory approach. One possible reason for this apparent bias is short-circuiting. Daisey and Hodgson (1989) observed a short-circuiting effect where the upstream concentration may be diluted by "cleaner" downstream air, which is in close proximity to the air cleaner inlet. This effect would tend to show a decreased removal efficiency of chemical based on the concentration at a room location away from the air cleaner, *e.g.* the center of the room. However, in general, the air cleaner upstream concentration was very similar to the room center concentration indicating a uniform concentration at least between those two points. Another possibility is the proximity of the toluene source to both the air cleaner upstream sampling location and the room center location. If the source addition was causing increased concentrations at both locations, the result would be a lower mass removal rate predicted by the mass balance approach. Since the reason is still being investigated, the mass balance values are used for the remaining analyses.

Also in Table 2 are the effective cleaning rates (ECR) for the portable air cleaner. This number is the product of the portable air cleaner's airflow rate and single pass removal efficiency. In terms of mass removal, the effective cleaning rates ranged from 180 kg/h to 256 kg/h. Thus the portable air cleaner was 8.5 to 12 times more effective at removing toluene from the test house than the average ventilation removal rate of 21 kg/h. The air cleaner effectiveness was also calculated according to Equation 8 and the results are shown in the final column of Table 2. Air cleaner effectiveness for the PORT air cleaner ranged from 83 % to 95 % with an average of 91 % ($\pm$ 4.3 %).

As stated earlier, the experiments were designed to determine if selected field operating conditions had a significant impact on air cleaner performance. Scatter plots illustrating the impact of relative humidity, HAC fan usage, and location on the PORT cleaning performance are provided in Figure 5. The plots indicate that none of the tested factors appeared to have a significant effect on the PORT removal efficiency for these tests. A regression analysis with just these variables also showed no significant effect. However, there were other variables (e.g., temperature and air change rate) that could not be controlled for these tests that may influence the factor analysis. A regression model including temperature and the original three factors (HAC status, relative humidity and room location) showed temperature to have a significant ($p < 0.05$) effect on removal efficiency, and a second regression analysis with an additional factor of air change rate showed relative humidity ($p < 0.05$) and air change rate ($p < 0.05$) to be significant. The difference in the models indicates that temperature may be confounded with relative humidity and air change rate, which is not an unexpected result. At best, these factor results are inconclusive, thereby requiring additional tests to verify these effects.

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Table 2. Portable Air Cleaner Results Summary

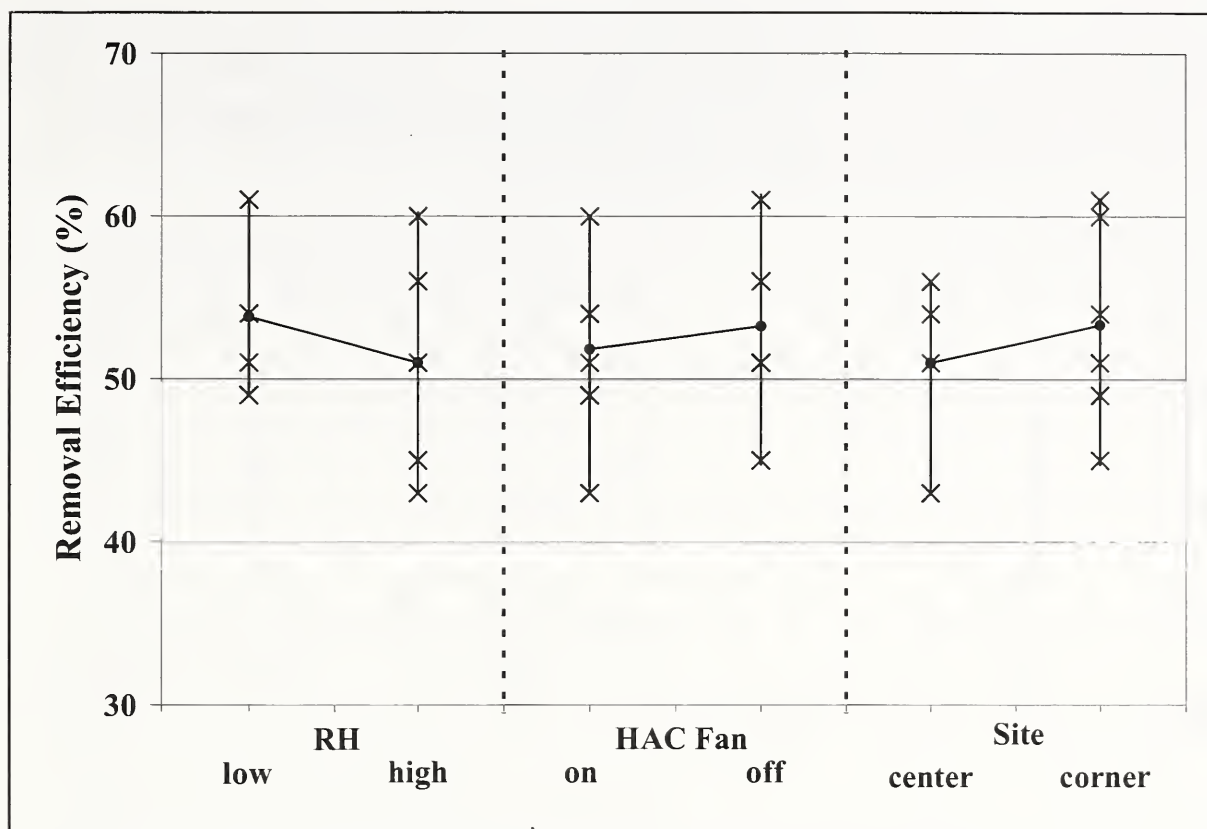| Expt. #	Location	HAC	Indoor Temp (°C)	Indoor R.H. (%)	Air change rate (h^{-1})	Direct		Mass Balance		ε (%)
						fdir(%)	ECR(m^3/h)	fmb(%)	ECR (m^3/h)	
PORT1a	center	on/ac	26 (±0.5)	n/a	0.11 (±0.02)	n/a	n/a	51 ± 1.5	177 ± 4.0	95
PORT1c	center	on/ac	29 (±0.3)	31 (±0.5)	0.13 (±0.003)	69 ± 1.6	241 ± 7.4	n/a	n/a	n/a
PORT1d	center	on/heat	30 (±0.1)	31 (±0.2)	0.18(±0.002)	65 ± 1.6	228 ± 7.3	54 ± 1.9	188 ± 5.5	93
PORT2	center	on/heat	28 (±0.3)	60 (±0.7)	0.22(±0.004)	77 ± 2.7	269 ± 11	43 ± 1.7	150 ± 9.9	83
PORT4	center	off	29 (±0.6)	55 (±0.9)	0.40 (±0.01)	68 ± 0.3	237 ± 4.9	56 ± 2.1	196 ± 6.2	85
PORT5a	corner	on/ac	29 (±0.3)	n/a	0.12 (±0.01)	68 ± 0.3	238 ± 4.9	49 ± 1.5	172 ± 4.0	94
PORT5b	corner	on/ac	29 (±0.1)	29 (±0.3)	0.11(±0.005)	n/a	n/a	54 ± 1.7	187 ± 4.8	95
PORT6	corner	on/heat	19 (±0.3)	62 (±0.3)	0.40 (±0.01)	77 ± 2.9	270 ± 11	60 ± 2.2	212 ± 6.3	86
PORT7	corner	off	24 (±0.1)	n/a	0.22 (±0.02)	65 ± 4.8	227 ± 17	61 ± 5.5	213 ± 19	92
PORT8a	corner	off	33 (±0.3)	40 (±0.2)	0.15 (±0.02)	n/a	n/a	45 ± 1.5	157 ± 4.2	92
PORT8b	corner	off	32 (±0.7)	57 (±2.5)	0.23 (±0.01)	59 ± 5.2	205 ± 19	51 ± 2.0	180 ± 6.1	90
					TOTAL AVERAGE:	70	243	55	191	91
					TOTAL STD DEV:	6.6	23	9.0	32	4.3

Figure 5. Portable air cleaner factor analysis for mass balance results.

In-Duct Air Cleaner

The single pass removal efficiency for the in-duct air cleaner was measured directly using upstream and downstream measurements and using the mass balance approach (see Table 3). For direct measurements, the average removal efficiency (f_{dir}) was 32 % (SD: 8.6 %) and ranged from 16 % to 44 %. The mass balance approach yielded an average removal efficiency (f_{mb}) of 41 % (SD: 12 %) and ranged from 26 % to 58 %. Over half the DUCT cases resulted in a higher removal efficiency predicted by the mass balance method than the direct measurement. Interestingly, this trend is opposite to what was observed by the PORT air cleaner. However, for this air cleaner, the difference between the mass balance results and the direct measurement results are within the uncertainty estimate. For consistency, the mass balance values are used for the remaining analyses. The effective cleaning rates in terms of mass ranged from 116 kg/h to 281 kg/h. These values are equivalent to a DUCT air cleaner effectiveness of 69 % to 93 % with an average of 86 % (SD: 6.8 %).

Factors for the DUCT air cleaner included relative humidity and the use of air conditioning vs. heat while the HAC fan was on. A scatter plot illustrating the impact of these factors on air cleaner performance is shown in Figure 6. For the DUCT air cleaner, relative humidity appeared to have an impact on performance, whereas the use of air conditioning or heating did not. However, an ANOVA analysis showed both relative humidity ($p < 0.001$) and the use of air conditioning or heat ($p < 0.01$) to be significant. In addition, the interaction between these two factors was also found to be significant ($p < 0.01$).

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Unlike the PORT air cleaner, the DUCT air cleaner removal efficiency tended to decrease with higher relative humidity. As discussed in the literature review, a relative humidity effect could be expected for both air cleaners. It is possible that since the relative humidity was always below 70 %, the PORT air cleaner may contain a large enough pore volume to absorb the extra water in addition to the toluene, whereas the DUCT air cleaner did not.
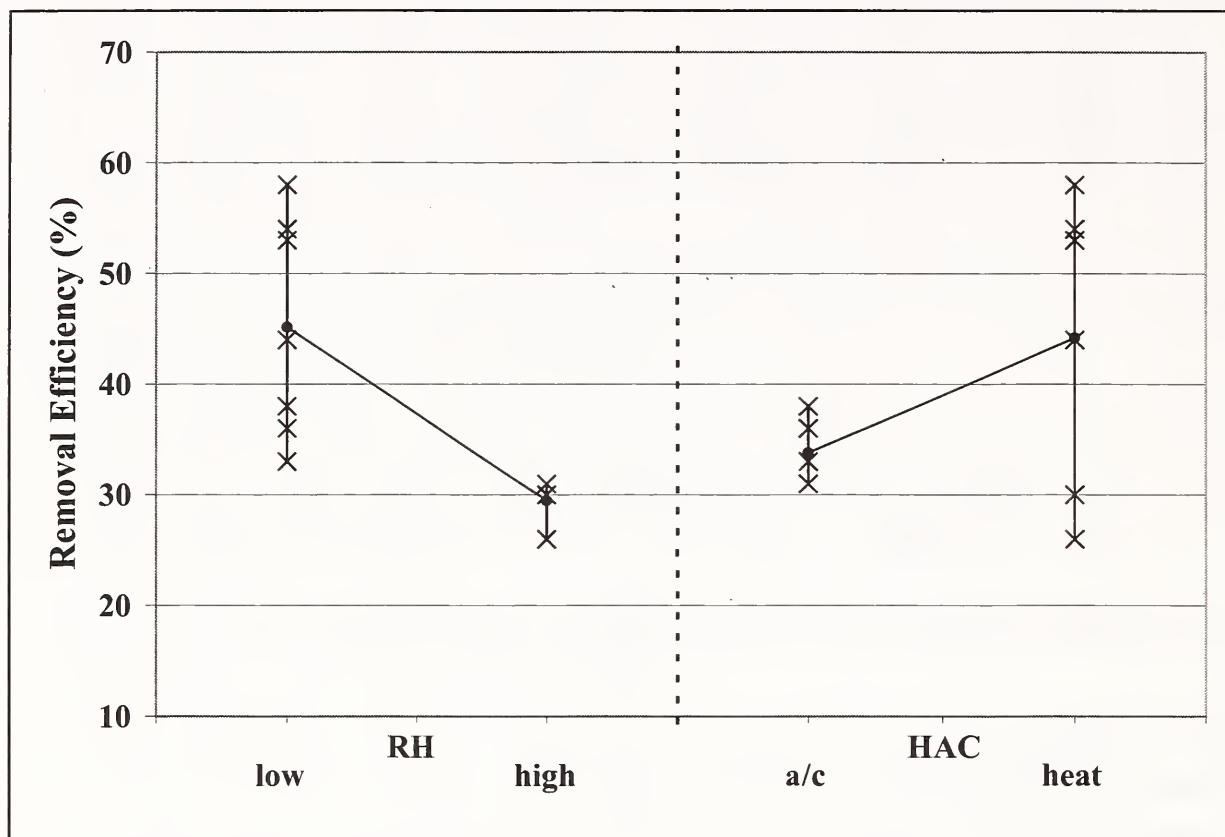

Figure 6. In-duct air cleaner factor analysis for mass balance results.

Table 3. In-Duct Air Cleaner Results Summary

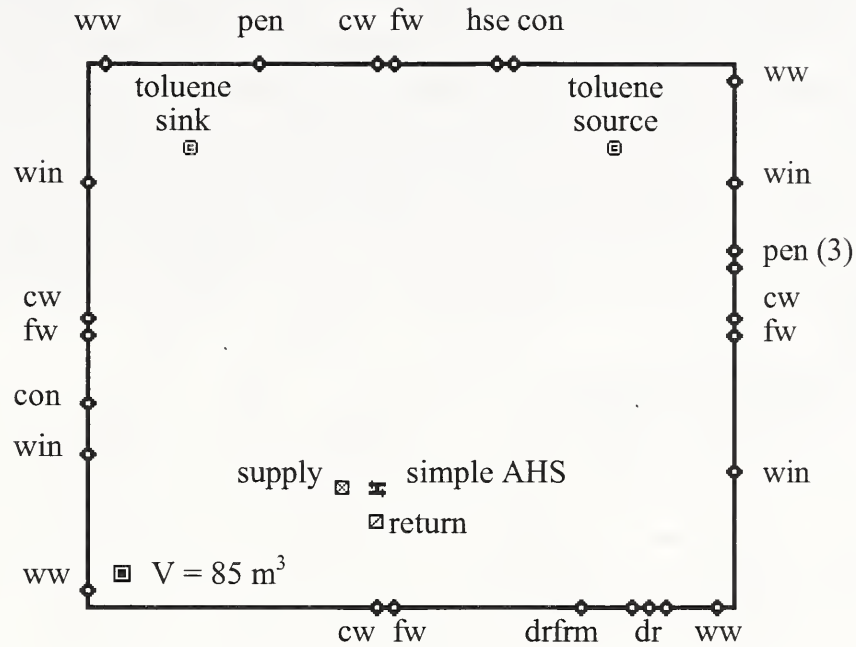| Expt. #	HAC	Indoor Temp (°C)	Indoor R.H. (%)	Air change rate (h^{-1})	Direct		Mass Balance		ε (%)
					fdir (%)	ECR (m³/h)	fmb (%)	ECR (m³/h)	
DUCT1a	on/ac	27 (±0.4)	27 (±0.4)	0.23 (±0.02)	42 ± 1.5	172 ± 6.7	33 ± 1.2	135 ± 4.1	87
DUCT1b	on/ac	26 (±0.3)	27 (±0.4)	0.14 (±0.02)	31 ± 2.0	127 ± 8.3	36 ± 1.2	146 ± 3.9	92
DUCT1c	on/ac	24 (±0.3)	36 (±0.5)	0.18 (±0.03)	29 ± 4.7	105 ± 17	38 ± 2.3	138 ± 8.0	90
DUCT2a	on/ac	22 (±0.3)	40 (±0.5)	0.20 (±0.0)	23 ± 4.7	82 ± 17	31 ± 2.0	113 ± 6.9	87
DUCT2b	on/ac	28 (±0.3)	40 (±0.5)	0.24 (±0.002)	16 ± 4.8	56 ± 17	31 ± 1.5	107 ± 4.7	84
DUCT3a	on/heat	26 (±0.5)	n/a	0.18 (±0.02)	n/a	n/a	54 ± 1.8	195 ± 5.4	93
DUCT3b	on/heat	22 (±0.6)	n/a	0.22 (±0.004)	34 ± 5.9	125 ± 22	53 ± 4.7	191 ± 17	91
DUCT3c	on/heat	20 (±0.2)	22 (±0.2)	0.47 (±0.03)	38 ± 4.1	151 ± 17	58 ± 5.5	234 ± 22	85
DUCT3d	on/heat	23 (±0.1)	31 (±0.2)	0.39 (±0.02)	44 ± 4.7	164 ± 18	44 ± 2.0	164 ± 6.7	83
DUCT4a	on/heat	19[a]	60[a]	0.32[a]	35 ± 6.9	133 ± 27	30 ± 1.3	117 ± 4.3	81
DUCT4b	on/heat	21 (±0.2)	62 (±0.7)	0.51 (0.05)	26 ± 3.5	99 ± 13	26 ± 1.6	97 ± 5.8	69
				AVERAGE:	32	122	41	155	86
				STD DEV:	8.6	37	12	46	6.8

SIMULATION RESULTS

A primary objective of this project was to determine the capability of CONTAM to predict the impact of a portable and in-duct gaseous air cleaner in the field. To meet this goal, a model of the test house, previously developed by Emmerich and Nabinger (2001), was updated to reflect recent changes to the building envelope. These changes, however, did not have a significant impact on the model's airflow characteristics. The fan pressurization test for the modified CONTAM model used in this study resulted in an air change rate of 7.4 h^{-1} at 50 Pa and an effective leakage area of 139 cm^2 at 4 Pa. These results are consistent with the measured fan pressurization test results by Emmerich and Nabinger (2001) (air change rate of 7.3 h at 50 Pa and effective leakage area of 140 cm^2).

A sketch of the CONTAM project file is provided in Figure 7. The model accounts for leakage in both the main level and attic. A summary of the model elements is provided in Table 4. Most of the leakage elements were found in ASHRAE Fundamentals Handbook (2001). The contaminant source was based on the measured value for each test, and the sink parameters were described in an earlier section. The house uses a recirculating air handling system (AHS), which is modeled with one supply (0.097 m^3/s) and one return (0.097 m^3/s) in the main level. The air cleaners were entered as part of the AHS with a removal rate equivalent to the experimentally determined removal efficiencies. These specific values will be presented for each model validation case.

Table 4. Model Elements shown in Figure 7.

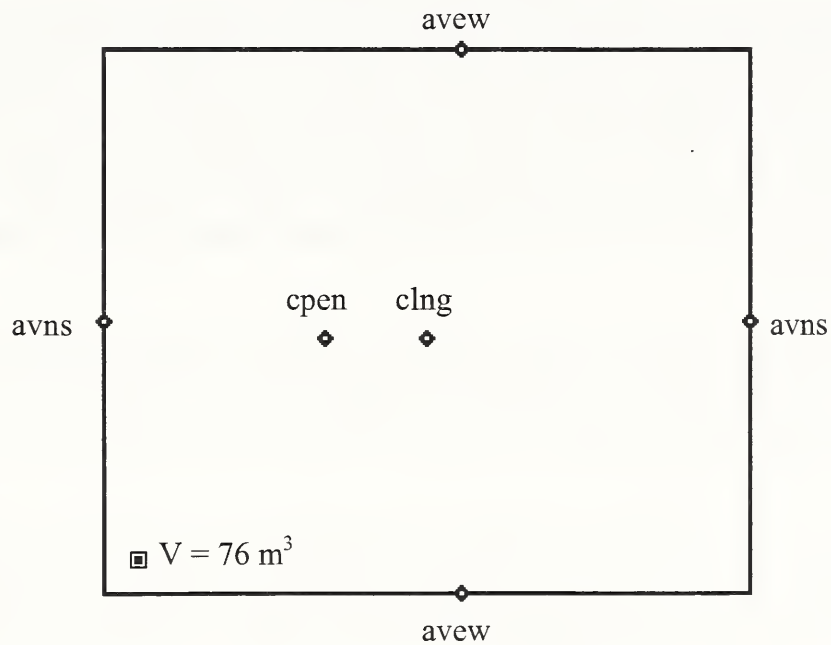| Airflow Element	Element Description	Effective Leakage Area at 4 Pa
avew	attic vent (on E and W walls)	0.061 m^2
avns	attic vent (on N and S walls)	0.045 m^2
clng	ceiling	0.908 cm^2/m^2
con	small conduit	0.2 cm^2
cpen	ceiling penetration	2.13 cm^2
cw .	ceiling-wall joint	0.864 cm^2/m
dr	door (distributed at 3 locations vertically)	21 cm^2
drfrm	door frame	1.7 cm^2/m^2
fw	floor-wall joint	2.08 cm^2/m
hse	hose penetration	0.5 cm^2
pen	wall penetration	1.3 cm^2
win	window	3.37 cm^2
ww	wall-wall joint	0.864 cm^2
Contaminant Element	**Model Input Parameters**	**Input Values**
Source	generation rate	21.6 mg/h
Sink	film mass transfer coefficient	0.068 m/h
	surface mass	1000 kg
	partition coefficient	0.00001
Simple AHS	Supply	0.097 m^3/s
	Return	0.097 m^3/s

Main Level:

Attic Level:

Figure 7. CONTAM sketchpad representation of test house (model elements are labeled with abbreviations used in Table 4).

A total of five air cleaner performance tests were completed for the simulation phase and are summarized in Table 5. Each test included measurements collected during different air cleaner operation scenarios and CONTAM simulations based on those conditions. Measured data collected for each test and used in the model included: ambient weather conditions, toluene emission rate from compressed gas cylinder, outdoor toluene concentrations, indoor temperature, and HAC duct airflow rate (for DUCT air cleaner). These data were collected in the same manner as described in the experimental section of this report. The air cleaner removal efficiency was based on the average of values determined in the experimental phase of this project (*i.e.*, not from the simulation test itself). Model performance was evaluated based on air change rates (calculated using SF_6 measured concentrations) and toluene concentrations measured in the center of the house.

Table 5. Air Cleaner Performance Tests

Case	Location	HAC	Temp (°C)	R.H. (%)	ACH (h^{-1})
PORT0215	center	on/heat	22 (± 0.5)	21 (± 0.4)	0.37 (± 0.04)
PORT0314	center	on/ac	18 (± 1.2)	40 (± 4.8)	0.20 (± 0.05)
DUCT0301	in-duct	on/heat	25 (± 1.2)	27 (± 1.8)	0.36 (± 0.02)
DUCT0306	in-duct	on/heat	21 (± 1.2)	22 (± 0.7)	0.25 (± 0.05)
DUCT0326	in-duct	on/heat	19 (± 0.6)	54 (± 2.8)	0.26 (± 0.05)

In order to accurately predict air cleaner performance, a model must also be able to adequately predict air change rates. As shown in the experimental results, air change rate does have a significant impact on contaminant removal from the indoor environment. A comparison of measured and predicted air change rates for the five tests is provided in Figure 8. The measured air change rates are based on ASTM E741 (ASTM 2001) as described in an earlier section. The predicted air change rates were based on model inputs of envelope leakage, indoor/outdoor temperatures, wind speed and wind direction. Both the measured and predicted values were based on 1 h averaging time.

For all five cases, the average absolute percent difference between measured and predicted air change rates was 15 % with the percent differences ranging from –21 % to 55 %. The case with the best agreement was DUCT 0326 with an average absolute percent difference between measured and modeled values of 9.3 %.

The predictive performance of CONTAM toluene concentrations was evaluated using ASTM D5157 guidelines (ASTM 2003). This guide provides statistical criteria for assessing the accuracy and bias of the model results compared to measured data. A summary of the suggested criteria and model results are given in Table 6.
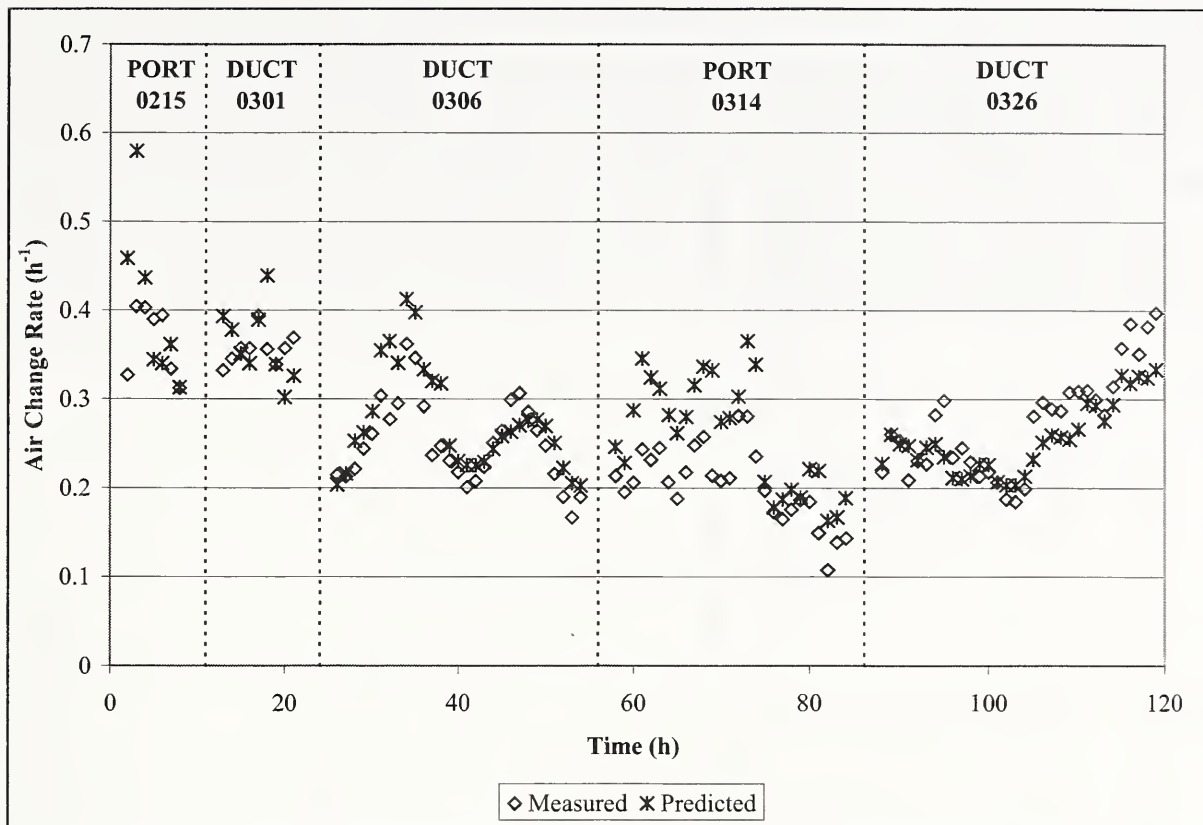
Figure 8. Comparison of measured and predicted air change rates for all five simulation tests.

Table 6. Statistical Parameters for Simulated and Measured Toluene Concentrations

Case	f^a (%)	$\overline{C_o}^b$ (mg/m³)	$\overline{C_p}^c$ (mg/m³)	R^d	b^e	$a/C_o (\%)^f$	$NMSE^g$	FB^h	FS^i
ASTM D5157 Criteria	n/a	n/a	n/a	> 0.9	0.75 < m < 1.25	< 25	< 0.25	< 0.25	< 0.5
PORT0215	55	0.092	0.087	0.997	0.93	1.7	0.0038	-0.056	-0.14
PORT0314	55	0.39	0.38	0.98	0.81	17	0.0089	-0.025	-0.31
DUCT0301	41	0.099	0.12	0.99	1.4	-12	0.048	0.23	0.64
DUCT0301*	52	0.099	0.10	0.99	1.1	-1.3	0.0029	0.046	0.13
DUCT0306	41	0.61	0.57	0.96	0.82	13	0.016	-0.054	-0.31
DUCT0306*	52	0.61	0.55	0.99	0.85	5.5	0.015	-0.095	-0.29
DUCT0326	41	0.50	0.64	0.98	1.2	13	0.071	0.24	0.33
DUCT0326*	28	0.50	0.68	0.92	1.1	25	0.12	0.30	0.37

Shaded cells indicate a value outside criteria limits.

a: Used overall average removal efficiency except for cases with (*) where used removal efficiency for specific relative humidity and HAC conditions.
b: Average observed toluene concentration.
c: Average predicted toluene concentration.
d: Correlation coefficient for relationship between C_p and C_o.
e: Slope of line of regression between C_p and C_o.
f: Intercept of line of regression between C_p and C_o, normalized by the observed concentration.
g: Normalized mean square error indicating the prediction error relative to C_p and C_o.
h: Fractional bias of the average values of C_p and C_o.
i: Fractional bias of the variance of C_p and C_o.

Two simulation tests were conducted with the portable air cleaner. The first test, PORT0215, was conducted with the air cleaner operating continuously in the center of the room. The toluene source was turned on at the same time as the air cleaner and also operated continuously. Results are shown in Figure 9. Since the experiments did not reveal an impact of operating and environmental conditions on the PORT air cleaner, an overall average experimental removal efficiency of 55 % was used in the PORT simulations. The resulting predicted toluene concentrations compared well with the measured values as shown by the ASTM D5157 criteria in Table 6. All six criteria were met indicating the model adequately predicted the toluene concentration for this scenario.

Figure 9. Comparison of measured and predicted toluene concentrations for PORT air cleaner test (PORT0215).

The second PORT simulation test was PORT0314. For this test, the air cleaner was operated on a schedule that cycled between on and off several times during the test. The toluene source was left on continuously as in PORT0215. As shown in Figure 10, the model does quite well at predicting the toluene concentration. Again, all six of the ASTM D5157 criteria were met.
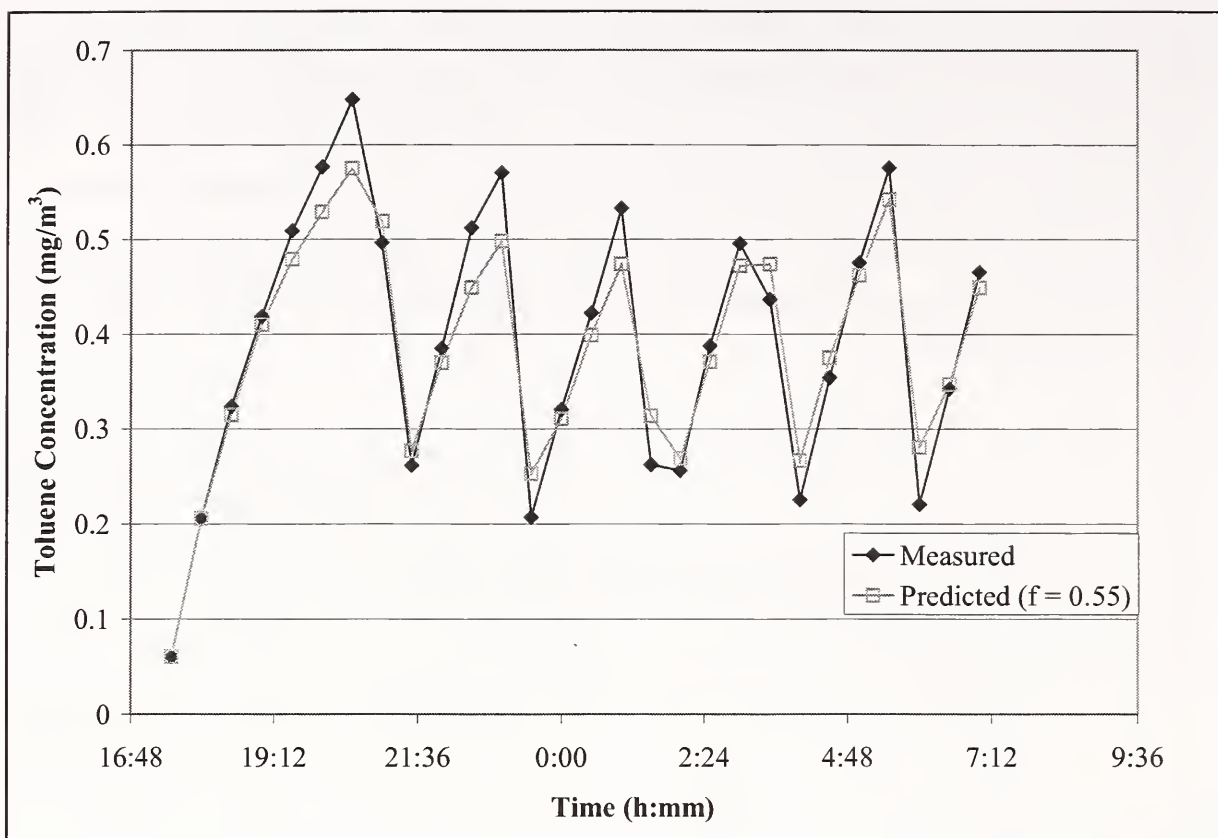
Figure 10. Comparison of measured and predicted toluene concentrations for PORT air cleaner test (PORT0314).

Three simulation tests were completed for the in-duct air cleaner. The first test, DUCT0301, was similar to PORT0215 with both the air cleaner and toluene source operating continuously (see Figure 11). Since the DUCT experiments showed a possible impact of relative humidity and HAC configuration (air conditioning vs. heat) on air cleaner performance, the model was run with two different removal efficiencies. A value of 41 % was used representing the average of all experimental air cleaner tests and a value of 52 % was the average of the experimental tests completed at low relative humidity with the heat on. Both results are shown in Figure 11, which illustrates the agreement of the measured and predicted concentrations with the low relative humidity removal efficiency. This agreement is further illustrated in Table 6 by the ASTM D5157 criteria. For a removal efficiency of 41 %, only four of the six criteria were met, whereas all six criteria were achieved for the removal efficiency of 52 %.

For test DUCT0306, the HAC fan was allowed to cycle on and off as controlled by the thermostat. Again, the toluene source was emitting continuously. This test was also completed at low relative humidity with the heat on. As a result, two model simulations were conducted, again using the overall average of 41 %, and the low relative humidity/heat on average of 52 %. This time, both removal efficiencies resulted in a reasonable match with the measured data. All six ASTM D5157 criteria were achieved for both cases. However, based on the criteria values and the data shown in Figure 13, the removal efficiency of 52 % resulted in a better match with measured toluene concentrations.
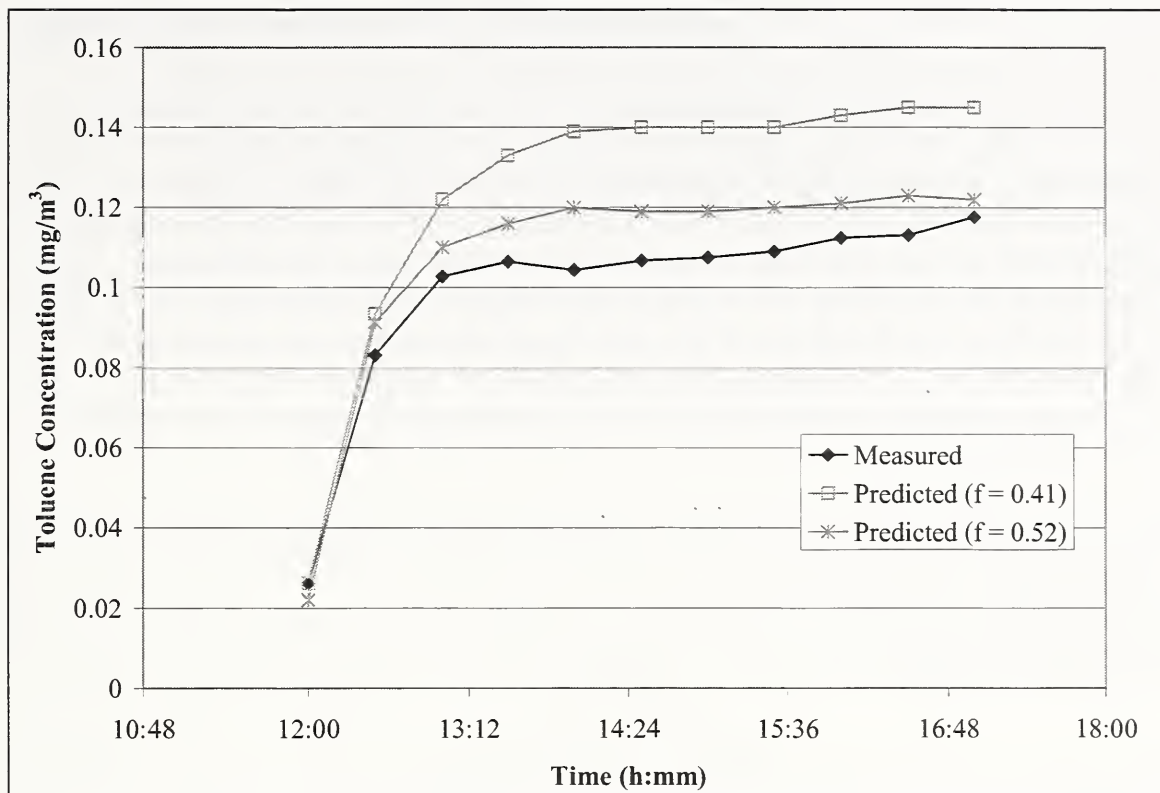
Figure 11. Comparison of measured and predicted toluene concentrations for DUCT air cleaner test (DUCT0301).
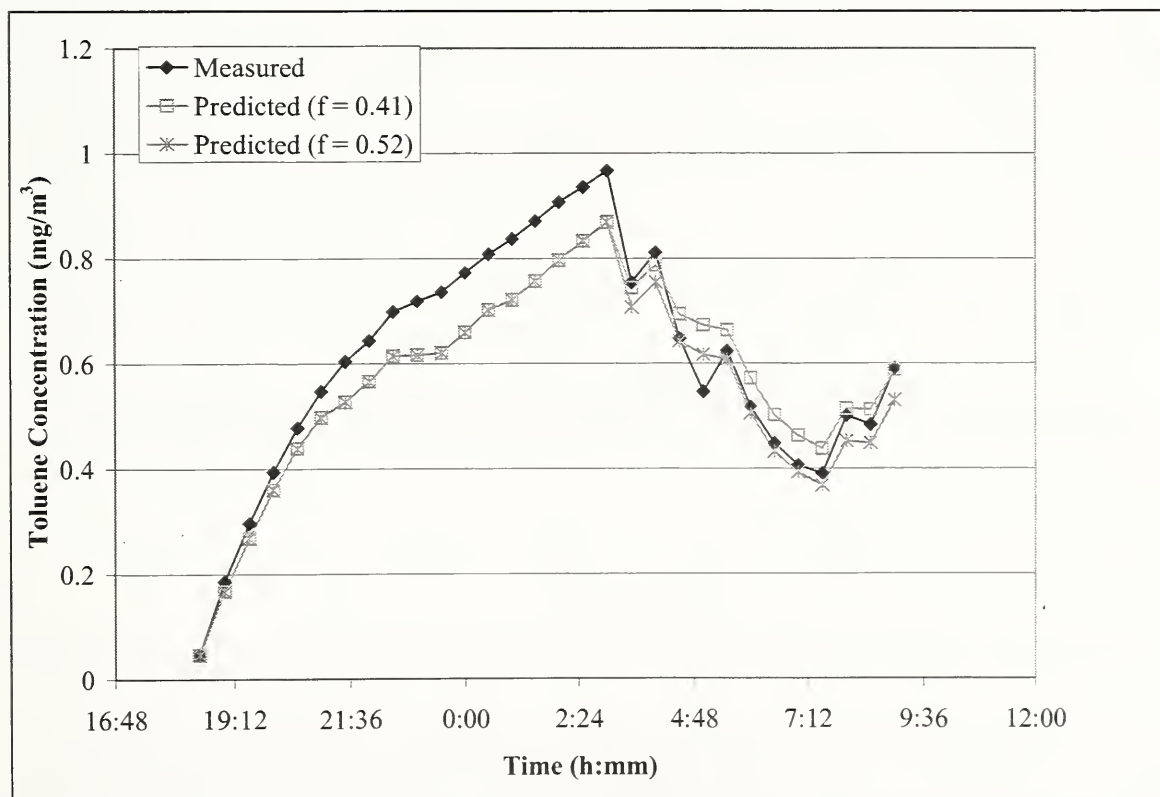

Figure 12. Comparison of measured and predicted toluene concentrations for DUCT air cleaner test (DUCT0306).

For simulation test DUCT0326, the HAC fan was allowed to cycle according to the thermostat with the toluene source on continuously. The relative humidity for this test was high (54 %). So, in addition to the overall average removal efficiency of 41 %, an average of 28 % based on heat on/high relative humidity experimental conditions was used for the simulation. The resulting measured and simulated data are shown in Figure 13. In this case, the removal efficiency specific to the operating/environmental conditions provided poorer agreement than the concentrations predicted by the overall average. For both cases, however, a large part of the difference may be due to the prediction of the air change rate and/or source emission rate rather than the air cleaner removal rate. During the initial four hours of this test, the air cleaner was not operating and the predicted and measured values are clearly building to a different steady-state value. This difference is not a result of the air cleaner removal efficiency, but does affect the comparison when the air cleaner is operating.
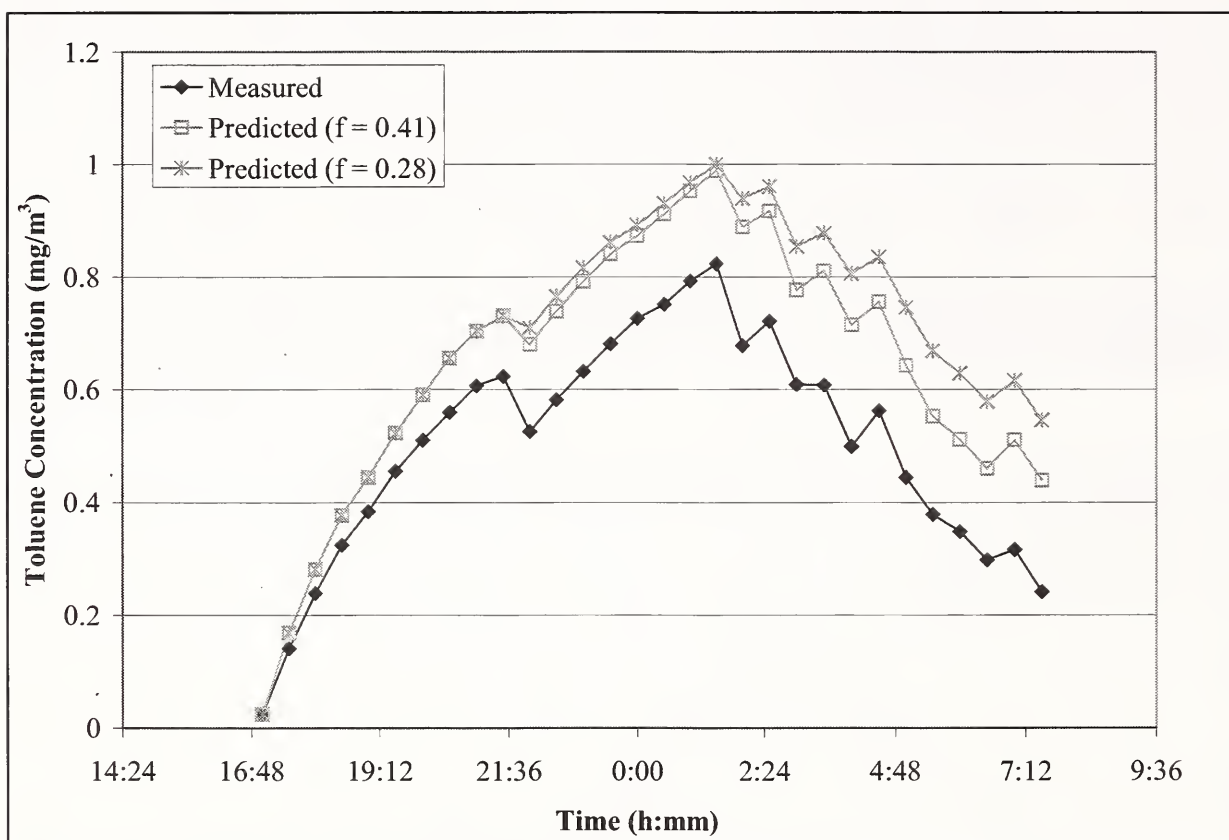

Figure 13. Comparison of measured and predicted toluene concentrations for DUCT air cleaner test (DUCT0326).

IMPACT OF GASEOUS AIR CLEANERS

Based on these results, CONTAM and other models should be able to provide a useful tool to evaluate the benefits of gaseous air cleaners and to compare air cleaner removal to other control strategies. For the five simulation tests, a scenario with no air cleaner was simulated. For test PORT0215 a steady-state toluene concentration of 0.6 mg/m^3 was reached with no air cleaner present compared to 0.1 mg/m^3 with the air cleaner on. Similarly for test PORT0301, a steady-state toluene concentration of 0.8 mg/m^3 was reached with no air cleaner compared to 0.15 mg/m^3 with the air cleaner operating. Thus, the PORT air cleaner provided an 83 % reduction in toluene concentration for the PORT0215 scenario and the DUCT air cleaner provided an 85 % reduction in toluene concentration for the DUCT0301 scenario.

Figure 14 shows the comparison of no air cleaner versus the PORT air cleaner for simulation test PORT0314. Even with the air cleaner cycling on and off, the peak toluene concentrations for this case never exceed 0.6 mg/m^3. Whereas with no air cleaner present, the toluene concentration increases continuously, eventually reaching a steady-state value of 1.3 mg/m^3 (not shown in Figure 14). For this scenario, the PORT air cleaner would reduce a person's exposure to toluene by 50 % over the test period.
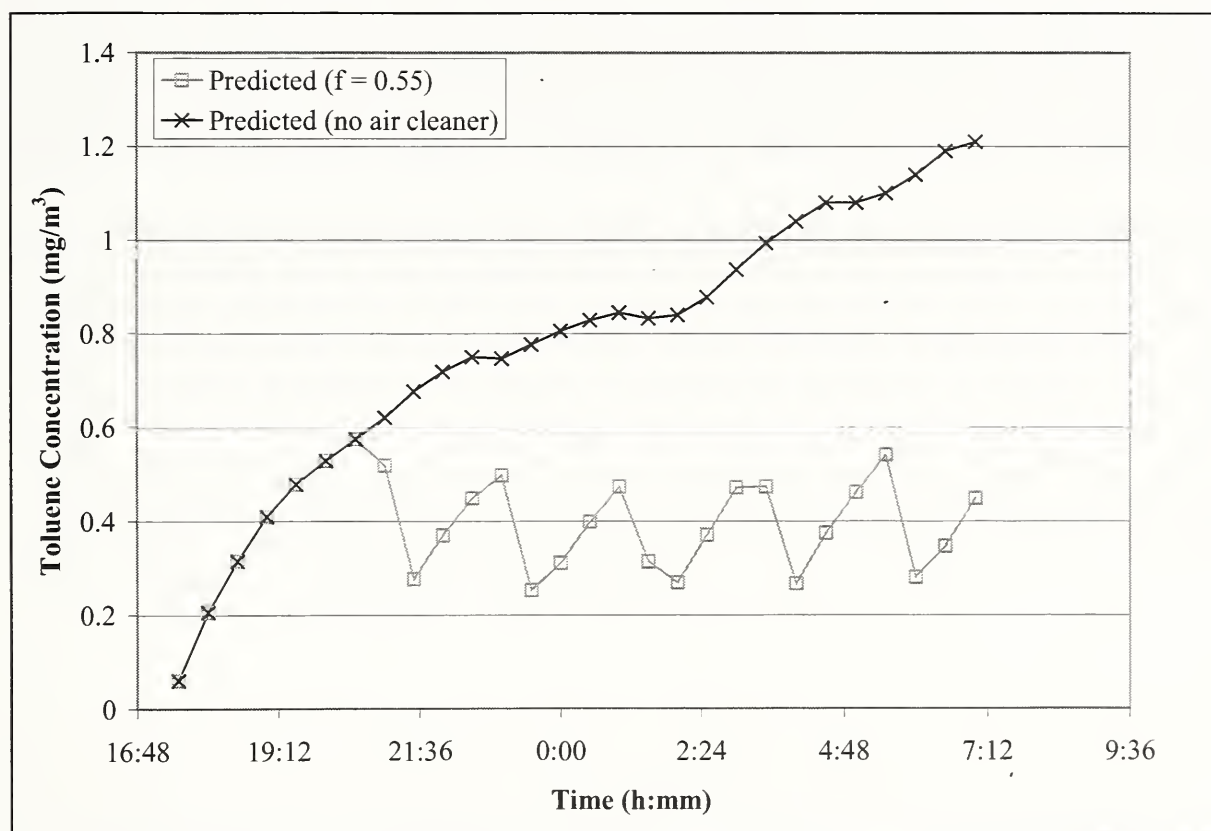

Figure 14. Comparison of PORT0314 simulated results with no air cleaner operating.

The impact of a particular air cleaner can also be compared with the impact of other control strategies including a different air cleaner or ventilation control. To show this comparison, a reference model of the test house was developed in CONTAM with a constant air change rate of 0.3 h^{-1}, constant sorption removal (as described earlier), a constant source of toluene (10 mg/h),

and no air cleaner operating. The resulting steady-state concentration for this reference case was 0.37 mg/m^3. If the air change rate was doubled for this case, the steady-state concentration was reduced to 0.20 mg/m^3, a 46 % reduction. Alternatively, if the DUCT air cleaner with a removal efficiency of 41 % was added to the reference case, the steady-state concentration was reduced to 0.059 mg/m^3, a reduction of 84 %. A comparison of the PORT and DUCT air cleaners showed that the PORT air cleaner's 14 % higher removal efficiency of 55 %, only resulted in a 4 % increase in toluene reduction (0.046 mg/m^3) due to the higher air flow rate of the DUCT air cleaner. In order to match the air cleaner effectiveness in this particular house, the air change rate would need to be as high as 2 h^{-1}.

DISCUSSION

Results from this work clearly showed the significant impact gaseous air cleaners can have on indoor contaminant concentrations. For all scenarios tested, the air cleaner was responsible for a majority of the contaminant removal, thereby reducing one's exposure at least 50 % more than infiltration alone, and often more than 90 %. Tests also revealed that both a portable and in-duct type of air cleaner would have a similar impact on toluene concentrations in a single zone environment. This result could change, however, in a multi-zone environment, where air cleaner location, volumetric flow rate, and air distribution could become more important.

This work also demonstrated the use of a mass balance method for testing gaseous air cleaners in the field. A dual phase experimental design in combination with semi-real time measurements allowed for the determination of material sink parameters as well as air cleaner removal rates. This method proved repeatable with the coefficient of variation for all replicate experiments less than 12 %. This approach resulted in different air cleaner removal efficiencies than those based on upstream and downstream measurements. Although this difference was not completely understood, it is possible that the placement of the upstream/downstream sample points led to more error in the direct removal efficiency value. Also, a measurement in the center of the room seemed to be more representative of the room concentration. As a result, the mass balance approach was deemed the most appropriate for measuring air cleaner removal in the field. The methods developed for these experiments will be carried over into the next phases of testing, including a second contaminant and a multi-zone building. Other future work needs include the ability to relate air cleaner laboratory performance to field performance to a mathematical model.

CONTAM performed well in predicting toluene concentrations in the single zone environment and is a potentially useful tool to demonstrate the benefits of air cleaning technologies. Concentrations predicted by CONTAM consistently met the ASTM D5157 statistical evaluation criteria when compared with measured values. While CONTAM is an effective tool for the specific scenarios described in this report, it is limited by the theory on which it is based, in particular the specific models of air cleaning used in the program. For example the model uses a constant removal efficiency, when in reality air cleaner performance can degrade over time and is dependent on environmental conditions that can change over time as well. As a result, there is a need to develop dynamic air cleaner models that allow for different conditions, including relative humidity, temperature, and face velocity.

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REFERENCES

Alberici, R.M., Jardim, W.F. (1997) "Photocatalytic destruction of VOCs in the gas-phase using titanium dioxide," *Applied Catalysis B: Environmental*, **14**: 55 - 68.

ASHRAE (2001) *ASHRAE Handbook – Fundamentals*, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA.

ASHRAE (2003) *ASHRAE Handbook - HVAC Systems and Equipment*, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA.

ASTM (2003) *Standard Guide for Statistical Evaluation of Indoor Air Quality Models. D5157-97e1*; American Society for Testing and Materials.

ASTM (2001) *Standard Test Method for Determining Air Change in a Single Zone by Means of a Tracer Gas Dilution. E741-00;* American Society for Testing and Materials.

Axley, JW. (1990) "Adsorption modeling for macroscopic contaminant dispersal analysis," NIST-GCR-90-573, National Institute of Standards and Technology, Gaithersburg, MD.

Blake, D.M. (1994) Bibliography of work on the photocatalytic removal of hazardous compounds from water and air, NREL/TP-430-6084. Published by the National Renewable Energy Laboratory, Golden, CO.

Boeniger, M.F. (1995) "Use of ozone generating devices to improve indoor air quality," *American Industrial Hygiene Association Journal*, **56**: 590 – 598.

Daisey, J.M. and Hodgson, A.T. (1989) "Initial efficiencies of air cleaners for the removal of nitrogen dioxide and volatile organic compounds," *Atmospheric Environment*, **23(9)**: 1885 - 1892.

Emmerich, S.J., and Nabinger, S.J. (2001). Measurement and simulation of the IAQ impact of particle air cleaners in a single-zone building. HVAC & R Research, 7 (3), 223 – 244.

Emmerich, S.J., Howard-Reed, C., Nabinger, S.J., Gupte, A., and Wallace, L. (2004). Measurement and simulation of the IAQ impact of particle air cleaners in a townhouse. In Preparation.

Fisk, W.J., Spencer, R.K., Grimsrud, D.T., Offermann, F.J., Pedersen, B., Sextro, R. (1987) *Indoor Air Quality Control Techniques - Radon, Formaldehyde, Combustion Products*, Noyes Data Corp., Park Ridge, New Jersey.

Godish, T. (1989) *Indoor Air Pollution Control*, Lewis Publishers, Inc., Chelsea, Michigan.

Jacoby, W.A., Blake, D.M., Fennell, J.A., Boulter, J.E., LeAnn M. Vargo, George, M.C., Dolberg, S.K. (1996) "Heterogeneous photocatalysis for control of volatile organic compounds in indoor air," *JAWMA*, **46**: 891 - 898.

Jacoby, W.A., Nimlos, M.R., Blake, D.M., Noble, R.D., Koval, C.A. (1994) "Products, intermediates, mass balances, and reaction pathways for the oxidation of trichloroethylene in air via heterogeneous photocatalysis," *Environmental Science & Technology*, **28**, 1661 - 1668.

Kagan, J. (1993) *Organic Photochemistry - Principles and Applications*, Academic Press Inc., San Diego, CA.

Lasdon, L.S., Waren, A.D., Jain, A., Ratner, M. (1978). "Design and testing of a generalized reduced gradient code for nonlinear programming," *ACM Transactions on Mathematical Software*, **4**(1), 34 - 49.

Lichtin, N.N., Sadeghi, M. (1998) "Oxidative photocatalytic degradation of benzene vapor over TiO_2," *Journal of Photochemistry and Photobiology A: Chemistry*, **113**, 81 - 88.

Lippmann, M. (1989) "Health effects of ozone - a critical review," *JAPCA*, **39**(5), 672 - 695.

Mahajan, B.M. (1987) "A method for measuring the effectiveness of gaseous contaminant removal devices - progress report," *NBSIR 87-3666*, U.S. Department of Commerce, National Bureau of Standards, Gaithersburg, MD.

Morrison, G.C., Nazaroff, W.W. (2002) "The rate of ozone uptake on carpet: Mathematical modeling," *Atmospheric Environment*, **36**, 1749 – 1756.

Nazaroff, W.W. (2000) "Effectiveness of air cleaning technologies," *Proceedings of Healthy Buildings 2000*, Vol 2, pp 49-54.

Nazaroff, W.W., Cass, G.R. (1986) "Mathematical modeling of chemically reactive pollutants in indoor air," *Environmental Science & Technology*, **20**, 924 – 934.

Obee, T.N., Brown, R.T. (1995) "TiO2 photocatalysis for indoor air applications: effects of humidity and trace contaminant levels on the oxidation rates of formaldehyde, toluene, and 1,3-butadiene," *Environmental Science & Technology*, **29**(5), 1223 - 1231.

Owen, M.K., VanOsdell, E.W., Jaffe, L.B., Sparks, L.E. (1995) "The effect of relative humidity on gaseous air cleaner media performance: toluene adsorption by activated carbon," In *Proceedings of Engineering Solutions to Indoor Air Quality Problems*, VIP-51, Air and Waste Management Association, Research Triangle Park, NC, pp. 551 - 562.

Shaughnessy, R.J., Levetin, E., Blocker, J., and Sublette, K.L. (1994) "Effectiveness of portable indoor air cleaners: sensory testing results," *Indoor Air*, **4**(3), 179 - 188.

Silberstein, S. (1991) "Proposed standard practice for assessing the performance of gas-phase air cleaning equipment," *NISTIR 4523*, National Institute of Standards and Technology, Gaithersburg, MD.

Stevens, L., Lanning, J.A., Anderson, L.G., Jacoby, W.A., Chornet, N. (1998) "Investigation of the photocatalytic oxidation of low-level carbonyl compounds," *JAWMA*, **48**: 979 - 984.

VanOsdell, D. (1994) "Evaluation of test methods for determining the effectiveness and capacity of gas-phase air filtration equipment for indoor air applications – Phase I: Literature review and test recommendations," *ASHRAE Transactions*, **100**, Pt. 2: 511 – 523.

VanOsdell, D.W., Owen, M.K., Jaffe, L.B., Sparks, L.E. (1996) "VOC removal at low contaminant concentrations using granular activated carbon," *JAWMA*, **46**: 883 - 890.

Weschler, C., Hodgson, A.T., and Wooley, J.D. (1992) "Indoor chemistry: ozone, volatile organic compounds, and carpets," *Environmental Science & Technology*, **26**: 2371 – 2377.

Weschler, C.J., Shields, H.C. (1997) "Potential reactions among indoor pollutants," *Atmospheric Environment*, **31**(21), 3487 - 3495.

Weschler, C.J., Shields, H.C., and Naik, D.V. (1994). Ozone-removal efficiencies of activated carbon filters after more than three years of continuous service. *ASHRAE Transactions*, **100**(2), pp. 1121 – 1129.

Zhang, J, Chen, Q, Zhang, J. (2001). "Modeling VOC sorption of building materials and its impact on indoor air quality," ASHRAE RP-1097. Atlanta: American Society of Heating, Refrigerating, and Air Conditioning Engineers, Inc.